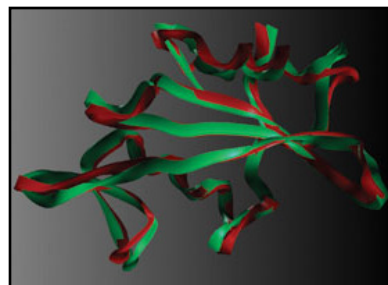


MODELING PROTEINS FROM SEQUENCE TO STRUCTURE

This course focuses on building 3D protein models from sequences and evaluating these models. Participants will search a database to find proteins that are homologous to a target sequence and use these homologous proteins as templates to construct a protein model of the target sequence. Learners will gauge the quality of the resulting protein model by examining its geometry and comparing it to other protein structures.



Who Should Attend

Modelers and structural biologists who require a 3D protein structure for continued studies. X-ray crystallographers and NMR spectroscopists who have insufficient data to determine a protein structure.

Requirements

Before attending this course, participants should be able to perform the following tasks in SYBYL: manipulate molecules with a mouse, and prepare protein structures. These topics are covered in the course [Protein Modeling for New Modelers](#).

What You Will Learn

- ▶ Create a 3D protein structure from your sequence for use in further molecular modeling studies.
- ▶ Derive reliable models from a high-quality, expansive database of protein structures.
- ▶ Measure the level of confidence you can place in your protein model.
- ▶ Detect distant homologs of the target sequence.
- ▶ Produce superior alignments based on structure and sequence information.

Course Topics

Align Sequences

- ▶ Find Homologous Protein Families

Model Proteins

- ▶ Model Conserved Regions
- ▶ Model Loops and Sidechains
- ▶ Evaluate Protein Model

Course Objectives

1. Identify protein templates for building a model of a target sequence.
2. Select appropriate homologs and build a model of the conserved regions.
3. Add appropriate loops and sidechains to the protein model.
4. Compare model to homologs and evaluate protein geometry.

Modules Used

SYBYL/Base, Biopolymer, and Advanced Protein Modeling (using FUGUE and ORCHESTRAR technologies).

Course Length

1 day

Schedule and Registration

For a schedule of Training Workshops and online registration, please visit

www.tripos.com/training